

Real root refinements for univariate polynomial equations

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ABSTRACT

Real root finding of polynomial equations is a basic problem in computer algebra. This task is usually divided into two parts: isolation and refinement. In this paper, we propose two algorithms LZ1 and LZ2 to refine real roots of univariate polynomial equations. Our algorithms combine Newton's method and the secant method to bound the unique solution in an interval of a monotonic convex isolation (MCI) of a polynomial, and have quadratic and cubic convergence rates, respectively. To avoid the swell of coefficients and speed up the computation, we implement the two algorithms by using the floating-point interval method in `Maple15` with the package `intpakX`. Experiments show that our methods are effective and much faster than the function `RefineBox` in the software `Maple15` on benchmark polynomials.

Keywords

Real root refinement, Newton's method, floating-point, interval method

1. INTRODUCTION

Solving for real solutions of univariate polynomial equations is a fundamental problem in computer algebra. Many other problems in mathematics or other fields can be reduced to it such as real solving multivariate polynomial equations [23, 6, 7, 5], studying the topologies of real algebraic plane curves [8], and generating ray-traced images of implicit surfaces in computer graphics [17]. There is a vast literature on calculating real zeros of univariate polynomials. We refer to [20] for some of the references.

The process of reliable computing real roots is usually divided into two steps: *real root isolation* (i.e., cutting the real axis so that each real root is contained in a separate interval) and *real root refinement* (i.e., narrowing each isolating interval to a given width). We mainly concerned with how to efficiently refine each real root of a univariate polynomial equation to a high precision. We propose two algorithms

LZ1 (Algorithm 3) and LZ2 (Algorithm 4) to refine real roots.

LZ1 is a combination of Newton's method and the secant method. It is based on Theorem 2.1 (cf. Theorem 4.6 in [34]) that can help choose a starting point and guarantee the quadratic convergence of the point sequence for Newton's method in an interval. By this theorem, all of the points in the sequence locate on the same side of the real root ξ , i.e., each point in the sequence provides a bound of ξ of the same kind (upper bound or lower bound). For each point in the sequence, to get a bound of ξ of the other kind, the secant method should be applied. Theorem 5.2 shows that LZ1 has an at least quadratic convergence rate.

LZ2 is also a combination of Newton's method and the secant method. But it makes an opposite choice of the starting point for Newton's method to LZ1. As a result, if we consider the starting point as a bound of ξ , then the point found by Newton's method becomes another bound of ξ of the other kind. After that, by the secant method, a new bound of ξ of the same kind with the starting point can be obtained. In this way, the two kinds of bounds of ξ arise alternately. Thus, the precision of each bound of ξ can benefit from its predecessor in this point sequence. So, it is not surprising that the sequence of inclusion intervals consisting of these bounds converges to ξ at least cubically (cf. Theorem 5.4).

However, the implementations of LZ1 and LZ2 will become slow if we evaluate polynomials in LZ1 and LZ2 exactly, since the representations of the numbers will swell dramatically. Fortunately, the floating-point interval method can help solve this problem. But this method can only deal with the so called well-posed problems in numerical computation. In fact, to apply this method to speed up the computation, we have already treated all the ill-posed cases by exact methods before calling LZ1 or LZ2.

To this aim, a square-free decomposition should be done first to get a list of square-free polynomials as components and to know the multiplicity of corresponding roots in each component. Then, we make a local monotonic convex decomposition (LMCD, cf. Definition 2) for each of these square-free polynomials to make sure each component has a monotonic convex isolation (MCI, cf. Definition 1). After that, based on existing methods for real root isolation [9, 2, 32, 24, 3, 19, 28, 4, 21], we compute a MCI for any polynomial in a LMCD of every square-free polynomial obtained in the first step. Finally, floating-point interval versions of LZ1 and LZ2 can be called safely in theory.

We have implemented LZ1 and LZ2 in `Maple15` with the

package `intpakX` which contains functions for floating-point interval computation in arbitrary precisions. Experiments were done on Chebyshev polynomials of the first kind to compare the efficiencies of LZ1, LZ2 and the `Maple` function `RefineBox`. The timings show that our implementations of LZ1 and LZ2 are much faster than `RefineBox` and that LZ2 is usually faster than LZ1.

Some variants of Newton's method also exist to reliably refine real roots of univariate polynomial equations.

Ramon E. Moore [18] in 1966 gave an interval Newton's method to compute a real root of a univariate real function in a closed interval. This method can be speeded up by using floating-point interval arithmetics [27]. It can give verified results, but sometimes it may fail, e.g. the resulting interval may contain the original one.

George E. Collins and Werner Krandick [11] in 1993 presented three versions of a variant of Newton's method and proved that the exact version has quadratic convergence rate. Among the three algorithms, they showed that the one using floating-point interval arithmetics performed much efficiently than the other two. Note that the restrictions of the input inclusion interval and the selection of the starting point for Newton's method in the exact version of their method are also the same with that in Theorem 2.1. But instead of a secant, when it is needed in LZ1, they used the line parallel to the tangent at the point that Newton's method is applied. Moreover, their method needs the input interval to satisfy a "3/4-assumption" to get started.

John Abbott [1] in 2006 proposed an algorithm named QIR. Then, based on the QIR, Michael Kerber and Michael Sagraloff [15] in 2011 gave an algorithm EQIR and analyzed its bit complexity. QIR and EQIR are combinations of the secant method and the bisection method. One feature of them is that they do not need any information of derivatives.

The rest of the paper is structured as follows. In Section 2, we introduce the basic theorem that LZ1 is based on. Section 3 is devoted to describing how multiplicities and the square-free polynomial components should be calculated. The notions of MCI and LMCD are given in Section 4 in order to get the intervals that can be used as inputs of LZ1 and LZ2. In Section 5, the main algorithms LZ1 and LZ2 are presented and their superlinear convergence properties are proved. Then we discuss how to use floating-point interval method to speed up LZ1 and LZ2 in Section 6. At last we make comparisons on efficiency among LZ1, LZ2 and the `Maple` function `RefineBox` in Section 7.

2. BASICS

This section is about a theorem which provides the basis of Algorithm 3 named LZ1 in Section 5.

Newton's method is a fast algorithm for computing solutions of equations. For a function and a starting point, generally, it is not easy to determine whether Newton's method converges or not. However, for univariate real functions there exists such a theorem as follows (cf. Theorem 4.6 in [34] written by Qingjin Yan in 1992).

THEOREM 2.1. *If a function $f \in C^2[a, b]$ and satisfies the following conditions:*

1. $f(a)f(b) < 0$;
2. the sign of $f''(x)$ does not vary on $[a, b]$;

3. $f'(x) \neq 0$ when $x \in [a, b]$;

4. $x_0 \in [a, b]$, $f(x_0)f''(x_0) > 0$,

then the sequence $\{x_k\}$ generated by

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, k = 0, 1, \dots$$

monotonically converges to the unique real root of $f(x) = 0$ in $[a, b]$ and the convergence rate is at least 2.

REMARK 2.2. *Note that the second condition of Theorem 2.1 allows $f''(x)$ to reach zero when $x \in [a, b]$. If we restrict this condition to " $f''(x) \neq 0$ when $x \in [a, b]$ ", then the iteration sequence will strictly monotonically converges.*

3. MULTIPLICITIES

We briefly recall how to compute multiplicities of roots of polynomial equations by existing methods.

Though numerical tools exist (e.g. [29, 16]) for computing multiplicities of roots of polynomial equations and most probably their outputs are correct, it is still possible that they output incorrect results sometimes. In other words, for a univariate polynomial $f \in \mathbb{Q}[x]$, computing the multiplicities of real or complex roots of the equation $f = 0$ is an ill-posed problem in numerical computation [27].

Thus, to know these multiplicities exactly, we should use exact methods. We can make a square-free decomposition of f such that there exist s polynomials g_1, \dots, g_s in $\mathbb{Q}[x]$ with $f = g_1^{r_1} \dots g_s^{r_s}$ where $1 \leq r_1 < \dots < r_s \leq n$ and $(g_i, g_j) = 1$ when $i \neq j$. Then $f = 0$ has a (complex or real) root ξ with multiplicity r if and only if there exists a polynomial g_i in the square-free decomposition of f such that $r = r_i$ and ξ is a single root of $g_i = 0$. The square-free decomposition of a univariate polynomial is easy to compute in the software `Maple15` with the function `sqrfree`. A factorization with the function `factor` in the same software can also help find the multiplicities of corresponding polynomial zeros. In practice, a square-free decomposition or a factorization costs much less time than real root isolations and refinements and can help reduce a reducible polynomial in $\mathbb{Q}[x]$ with high degree to some lower degree polynomials which are relative easier to deal with.

In the rest of this paper, we assume that f is a square-free polynomial with rational coefficients.

4. MONOTONIC CONVEX ISOLATIONS

To refine a real root of a square-free polynomial $f \in \mathbb{Q}[x]$, it should be first isolated from other real roots. In this section, we give a concept called monotonic convex isolation (Definition 4.1). If f has such an isolation, then any real root of f is contained in a closed interval where the monotonicity and convexity of f is fixed unless the interval is a point. The refinements of real roots in the next section will benefit a lot from the properties of monotonicity and convexity of f on these isolating intervals. However, certain square-free polynomials in $\mathbb{Q}[x]$ have no monotonic convex isolations. In this case, we want to decompose f to a multiplication of some polynomials that have monotonic convex isolations (Theorem 4.5). This leads to the concept of local monotonic convex decomposition (Definition 4.4). At the end of this section, we give an algorithm to compute such a decomposition.

DEFINITION 4.1 (MCI). *Given a real root isolation Iso of a square-free polynomial $f \in \mathbb{Q}[x]$, we say that Iso is a monotonic convex isolation of f if $I \in Iso$ is not a point implies that $f'(x) \neq 0$ and $f''(x) \neq 0$ for all $x \in I$.*

REMARK 4.2. “ $I \in Iso$ is not a point” in the above definition means that the closed interval I is not in the form of $[a, a]$ where a is a rational number. Note that such stuff may exist in Iso .

If f has a MCI, then we can work it out by Algorithm 1. Note that Algorithm 1 is not a definite algorithm but a description of a class of algorithms. When the base algorithm for real root isolation (e.g. the RS C-library [22, 23, 24] of Fabrice Rouillier and DISCOVERER [30, 31] of Bican Xia) is chosen, then Algorithm 1 will become definite. Hence, its efficiency mainly depends on the chosen base algorithm.

Algorithm 1: MCI

- Data:** A polynomial $f \in \mathbb{Q}[x]$ that has a MCI
Result: A monotonic convex isolation of f
- 1 Compute a real root isolation Iso of f in common sense by a base algorithm.
 - 2 For each interval $I \in Iso$ that is not a point, cut I by bisection method and consider the sign of the value of f at the midpoint of I to find the interval that contains the real root in I (sometimes, the midpoint is just the real root).
 - 3 Repeat step 2 until neither f' nor f'' has real roots in the resulting closed interval I^* (this can be done by using inclusion and exclusion criteria).
 - 4 Return the set consisting of all the I^* in step 3 and all the point intervals arising in Iso or during the computation of step 3.
-

It is obvious that for a nonconstant square-free polynomial f , if it satisfies $(f, f'') = 1$ then f has a MCI. However, not all real polynomials have monotonic convex isolations. We give a counterexample below.

EXAMPLE 4.3. *Pick f as $x(x+1)(x+2)$. Then $f' = 3x^2 + 6x + 2$ and $f'' = 6(x+1)$. It is easy to see that -1 is the common real root of f and f'' . Obviously, f has no MCI.*

Hence, we want a decomposition of f such that each component has a MCI. This idea delivers the following definition.

DEFINITION 4.4 (LMCD). *If a square-free polynomial $f \in \mathbb{Q}[x]$ can be represented as the multiplication of s polynomials g_1, \dots, g_s where $\deg(g_i) = 1$ or $\gcd(g_i, g_i'') = 1$ for every $i = 1, \dots, s$, then we say that f has a local monotonic convex decomposition.*

THEOREM 4.5. *Every nonconstant square-free polynomial $f \in \mathbb{Q}[x]$ has a local monotonic convex decomposition.*

PROOF. For a polynomial $f \in \mathbb{Q}[x] \setminus \mathbb{Q}$, we prove the theorem by induction on the degree d of f .

When $d = 1$, the theorem holds obviously. Supposing the conclusion of the theorem holds when $d \leq k$ ($k \geq 1$), we prove that it also holds for $d = k+1$. Denote $g := \gcd(f, f'')$. It is easy to see that $\deg(g) < \deg(f)$ when $d > 1$. If $g = 1$ then the conclusion holds. Otherwise, there exists

a polynomial $h \in \mathbb{Q}[x] \setminus \mathbb{Q}$ such that $f = gh$. Since $\deg(g)$ and $\deg(h)$ are all no larger than k , we know that g and h all have local monotonic convex decompositions by the induction assumption. Thus, f has a local monotonic convex decomposition.

Therefore, the conclusion of the theorem holds for all non-constant square-free polynomials in $\mathbb{Q}[x]$. \square

COROLLARY 4.6. *Any nonconstant irreducible polynomial $f \in \mathbb{Q}[x]$ forms a LMCD of itself.*

REMARK 4.7. *Sometimes, the irreducibility of a polynomial f in $\mathbb{Q}[x]$ is easy to test by certain irreducibility criteria, e.g. Eisenstein's criterion. If the irreducible decomposition of f in $\mathbb{Q}[x]$ is known, then it is also a monotonic convex decomposition of f according to Corollary 4.6.*

Based on the proof of Theorem 4.5, we give Algorithm 2 (LMCD) to compute a local monotonic convex decomposition of f . The termination and correctness are obvious and we omit the proofs. In most cases, the algorithm LMCD only tests that f and f'' are coprime. This test is usually very fast in practice.

Algorithm 2: LMCD

- Data:** A nonconstant square-free polynomial $f \in \mathbb{Q}[x]$
Result: A local monotonic convex decomposition of f
- 1 $S := \{\}$;
 - 2 **if** $\deg(f) = 1$ **then**
 - 3 $S := \{f\}$;
 - 4 **return** S ;
 - 5 **end**
 - 6 $g := \gcd(f, f'')$;
 - 7 **if** $g = 1$ **then**
 - 8 $S := \{f\}$;
 - 9 **return** S ;
 - 10 **end**
 - 11 $S := S \cup \text{LMCD}(g) \cup \text{LMCD}(f/g)$;
 - 12 **return** S ;
-

EXAMPLE 4.8. *For the polynomial $f = x^3 + 3x^2 + 2x$ in Example 4.3, it can be decomposed into two polynomials by Algorithm 2, i.e., the output is $\{x+1, x^2+2x\}$. For $x+1 = 0$, we can directly compute the root. For $x^2 + 2x$, it has a monotonic convex isolation.*

5. REAL ROOT REFINEMENTS

In this section, we study how Newton's method and the secant method can be combined and applied on the MCI intervals to compute narrower inclusion intervals of the real roots of a univariate polynomial equation. For this, we provide two algorithms LZ1 (Algorithm 3) and LZ2 (Algorithm 4), and prove that their convergence rates are at least 2 and 3, respectively.

We design LZ1 (Algorithm 3) based on Theorem 2.1. According to this theorem, the initial point x_0 for Newton's method should satisfy the condition $f(x_0)f''(x_0) > 0$, and the point sequence $\{x_i\}_{i=0}^{\infty}$ of Newton's method converges monotonically. This provides a series of bounds of the real root ξ on one side. Since the convexity does not change in the input MCI interval $[a, b]$, the secant method can be used

to obtain a bound c_{i+1} on the other side of ξ after getting each x_i by Newton's method. Then a sequence of inclusion intervals of ξ is obtained. Theorem 5.2 shows that this sequence converges at least quadratically.

The second main algorithm LZ2 (Algorithm 4) is also a combination of Newton's method and the secant method. In contrast to LZ1, the condition for selecting initial point c_0 for Newton's iteration in LZ2 is $f(c_0)f''(c_0) < 0$. As a result, the point $z(x_1)$ obtained by Newton's method on f at c_0 locates at the other side of ξ . Then we can get c_1 as a bound of ξ at the same side with c_0 by the secant method. In this way, the inclusion interval sequence of ξ can obtain an at least cubic convergence rate (cf. Theorem 5.4). However, note that when $z \notin [a, b]$, the behavior of f at z will be out of control. In this case, $[a, b]$ should be cut until the new z locates in the new initial MCI interval. This task is easy to do by using the secant method as described in lines 4-4 of Algorithm 4. Then the fast convergent iteration can start.

We want the outputs of LZ1 and LZ2 to be narrow intervals from which the precisions of the corresponding real roots can be read out directly. However, no matter how narrow an interval containing zero is, we cannot obtain any correct bits by comparing the two endpoints of the interval. Hence, LZ1 and LZ2 are not allowed to input intervals that contain zero. In fact, when a monotonic convex isolation of a square-free polynomial f is performed as we discussed in the last section, it is very easy to check whether $f = 0$ has zero solution or not. If such solution exists, its isolation interval can be set as the interval $[0, 0]$ in the MCI directly.

EXAMPLE 5.1. Given $L = 8$ (decimal digits), a square-free polynomial $f := x^3 - 20x + 7$ and an interval $[\frac{4389}{1024}, \frac{1097}{256}]$ in a monotonic convex isolation of f , we show the process of the iteration of Algorithm 3 as follows.

$$\begin{aligned} [a_0, b_0] &= [\frac{4389}{1024}, \frac{1097}{256}] \\ [a_1, b_1] &= [\frac{40379863349}{9422150912}, \frac{80788619485}{18851042816}] \\ [a_2, b_2] &= [\frac{18537520582609738516073933520140272183127}{4325505299448020965613362785214886187776}, \frac{503844952756268930733017297728389}{117566100791919345105185727965440}] \end{aligned}$$

$(b_2 - a_2)/b_2 \approx 0.6053885328 \times 10^{-14} < 10^{-8}$. Hence, the algorithm terminates and outputs $[a_2, b_2]$.

THEOREM 5.2. The iteration in Algorithm 3 converges and the convergence rate is at least 2.

PROOF. From the loop in lines 3-3 of Algorithm 3, we know that the iteration is

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \quad (1)$$

$$c_{i+1} = \frac{x_i f(c_i) - c_i f(x_i)}{f(c_i) - f(x_i)} \quad (2)$$

where x_i and c_i means the i -th iteration of x and c for $i = 0, 1, \dots$, respectively.

We first prove that the real root ξ of the equation $f = 0$ always lies in the open interval between x_i and c_i . By Theorem 2.1, we know that the sequence $\{x_i\}_{i=0}^{\infty}$ converges monotonically to ξ and that no x_i is equal to ξ . Thus, these

Algorithm 3: LZ1

Data: A closed interval $[a, b]$ ($ab > 0$ and $a < b$) in a monotonic convex isolation of a square-free polynomial $f \in \mathbb{Q}[x]$ and a positive integer L

Result: A closed interval $[a', b']$ such that the only real root ξ of $f = 0$ in $[a, b]$ is also in it and $(b' - a')/|\xi| \leq 10^{-L}$

```

1 if  $|b - a| \leq 10^{-L} \min(|a|, |b|)$  then
2   return  $[a, b]$ ;
3 end
4 if  $f(a)f''(a) > 0$  then
5    $x \leftarrow a$ ;  $c \leftarrow b$ ;
6 else
7    $x \leftarrow b$ ;  $c \leftarrow a$ ;
8 end
9 while  $|x - c| > 10^{-L} \min(|x|, |c|)$  do
10   $u \leftarrow f(x)$ ;
11   $v \leftarrow f(c)$ ;
12   $p \leftarrow x - u/f'(x)$ ;
13   $c \leftarrow (xv - cu)/(v - u)$ ;
14   $x \leftarrow p$ ;
15 end
16 return  $[\min(x, c), \max(x, c)]$ .
```

x_i 's are the bounds of ξ on the same side. We only need to prove that the c_i 's are the bounds of ξ on the other side and $c_i \neq \xi$. Note that if c_i and x_i are on different sides of ξ , then $f(c_i)/(f(c_i) - f(x_i))$ and $-f(x_i)/(f(c_i) - f(x_i))$ are all in $(0, 1)$ and their sum is 1. By induction on i , applying Jessen's inequality we have that $f(c_{i+1}) < 0$ when $f''(a) > 0$ and $f(c_{i+1}) > 0$ when $f''(a) < 0$, i.e.,

$$f(c_{i+1})f''(a) < 0;$$

consequently, c_{i+1} locates on the opposite side of x_{i+1} w.r.t. ξ and $c_{i+1} \neq \xi$. This proves that ξ always lies in the open interval between x_i and c_i .

Next, we study the convergence of the sequence consisting of the interval lengths. According to the Mean Value Theorem, there exist a $\lambda \in (\min\{x_i, \xi\}, \max\{x_i, \xi\})$ and a $\mu \in (\min\{c_i, x_i\}, \max\{c_i, x_i\})$ such that $f(x_i) = f'(\lambda)(x_i - \xi)$ and $\frac{f(c_i) - f(x_i)}{c_i - x_i} = f'(\mu)$. Note that the sequence $\{c_i\}_{i=0}^{\infty}$ converges to ξ monotonically. Indeed, since c_{i+1} and c_i are on the same side of ξ and

$$c_{i+1} - c_i = \frac{(x_i - c_i)f(c_i)}{f(c_i) - f(x_i)} = -\frac{f'(\tau)}{f'(\mu)}(c_i - \xi),$$

we know that $\{c_i\}_{i=0}^{\infty}$ is monotone and has a bound ξ . Then $\{c_i\}_{i=0}^{\infty}$ converges and it is easy to see the limit is ξ . Since there exists φ between c_i and x_i such that $f(c_i) = f(x_i) + (c_i - x_i)f'(x_i) + (c_i - x_i)^2 f''(\varphi)/2$, we have

$$\begin{aligned} x_{i+1} - c_{i+1} &= x_i - \frac{f(x_i)}{f'(x_i)} - \frac{x_i f(c_i) - c_i f(x_i)}{f(c_i) - f(x_i)} \\ &= f(x_i) \left(\frac{1}{\frac{f(c_i) - f(x_i)}{c_i - x_i}} - \frac{1}{f'(x_i)} \right) \\ &= \frac{f(x_i)f''(\varphi)}{2f'(\mu)f'(x_i)}(x_i - c_i) \\ &= \frac{f''(\varphi)f'(\lambda)}{2f'(\mu)f'(x_i)}(x_i - c_i)(x_i - \xi). \end{aligned}$$

From Definition 4.1 and the input of Algorithm 3, we know that $f'(\xi) \neq 0$ and $f''(\xi) \neq 0$. Hence,

$$\limsup_{i \rightarrow \infty} \frac{|x_{i+1} - c_{i+1}|}{|x_i - c_i|^2} \leq \left| \frac{f''(\xi)}{2f'(\xi)} \right| \neq 0.$$

Therefore, the sequence of the lengths of the intervals has at least quadratic convergence rate. \square

Algorithm 4: LZ2

Data: A closed interval $[a, b]$ ($ab > 0$ and $a < b$) in a monotonic convex isolation of a non-constant real univariate square-free polynomial f and a positive integer L

Result: A closed interval $[a', b']$ such that the only root ξ of $f = 0$ in $[a, b]$ is also in it and $(b' - a')/|\xi| \leq 10^{-L}$

```

1 if  $|b - a| \leq 10^{-L} \min(|a|, |b|)$  then
2   return  $[a, b]$ ;
3 end
4 if  $f(a)f''(a) > 0$  then
5    $x \leftarrow a$ ;  $c \leftarrow b$ ;
6 else
7    $x \leftarrow b$ ;  $c \leftarrow a$ ;
8 end
9  $u \leftarrow f(x)$ ;  $v \leftarrow f(c)$ ;
10  $z \leftarrow c - v/f'(c)$ ;
11 while  $z \notin [a, b]$  do
12    $c \leftarrow (xv - cu)/(v - u)$ ;
13    $v \leftarrow f(c)$ ;
14    $z \leftarrow c - v/f'(c)$ ;
15 end
16  $x \leftarrow z$ ;
17 while  $|x - c| > 10^{-L} \min(|x|, |c|)$  do
18    $u \leftarrow f(x)$ ;
19    $c \leftarrow (xv - cu)/(v - u)$ ;
20   if  $|x - c| \leq 10^{-L} \min(|x|, |c|)$  then
21     return  $[\min(x, c), \max(x, c)]$ ;
22   end
23    $v \leftarrow f(c)$ ;
24    $x \leftarrow c - v/f'(c)$ ;
25 end
26 return  $[\min(x, c), \max(x, c)]$ .
```

EXAMPLE 5.3. For the polynomial and the initial interval in Example 5.1, we apply Algorithm 4 to them and get the intermediate interval sequence (other than Example 5.1, the intervals renew only one endpoint each time):

$$\begin{aligned}
[a_0, b_0] &= \left[\frac{4389}{1024}, \frac{1097}{256} \right] \\
[a_0, b_1] &= \left[\frac{4389}{1024}, \frac{1261419417}{294336896} \right] \\
[a_1, b_1] &= \left[\frac{6671209230324943307293}{1556645655550311117184}, \frac{1261419417}{294336896} \right] \\
[a_1, b_2] &= \left[\frac{6671209230324943307293}{1556645655550311117184}, \right. \\
&\quad \left. \frac{283700456965465533230109 \dots 42 \text{ digits are omitted}}{66198056239039164770905 \dots 42 \text{ digits are omitted}} \right]
\end{aligned}$$

$(b_2 - a_1)/b_2 \approx 0.1438320660 \times 10^{-10} < 10^{-8}$. Hence, the algorithm Algorithm 4 terminates and outputs $[a_1, b_2]$.

THEOREM 5.4. The iteration in Algorithm 4 converges and the convergence rate is at least 3.

PROOF. The iteration in Algorithm 4 has two stages, i.e., the loops in lines 4-4 and in lines 4-4.

We first prove that the loop in lines 4-4 terminates. In this process, x is fixed. By Jessen's inequality, we have that $f(c_i)f''(a) < 0$ for the i -th iteration of c in this loop (cf. the proof of Theorem 5.2). Hence, these c_i 's all locate at the other side of x w.r.t. ξ and if the loop does not terminate the sequence consisting of them monotonically converges to ξ . Thus, the sequence $\{z_i\}_{i=0}^{\infty}$ will also converge to $\xi \in (a, b)$, a contradiction. Therefore, the loop in lines 4-4 terminates and the number of iterations is independent of L .

Next, we study the loop in lines 4-4 which is the iteration as

$$x_{i+1} = c_i - \frac{f(c_i)}{f'(c_i)} \quad (3)$$

$$c_{i+1} = \frac{c_i f(x_{i+1}) - x_{i+1} f(c_i)}{f(x_{i+1}) - f(c_i)} \quad (4)$$

where c_0 is the last value of c in the loop in lines 4-4 and x_0 is the x assigned in lines 4-4. Consequently, x_1 locates in the open interval between x_0 and ξ . By Jessen's inequality and from iteration (4) we know that c_1 locates in the open interval between c_0 and ξ . Note that the derivative of the function $x(t) := t - f(t)/f'(t)$ is $f(t)f''(t)/(f'(t))^2$ and that $f(c_0)f''(c_0) < 0$. By induction on i , it is not difficult to see that the two sequences $\{x_i\}_{i=0}^{\infty}$ and $\{c_i\}_{i=0}^{\infty}$ all monotonically converge to ξ but from opposite directions. This proves that the iteration in Algorithm 4 converges to ξ .

At last, we study the convergence rate of this iteration. It is in fact the convergence rate of the second stage, i.e., the loop in lines 4-4. Then we have that

$$\begin{aligned}
x_{i+1} - c_{i+1} &= c_i - \frac{f(c_i)}{f'(c_i)} - \frac{c_i f(x_{i+1}) - x_{i+1} f(c_i)}{f(x_{i+1}) - f(c_i)} \\
&= f(c_i) \left(\frac{1}{\frac{f(x_{i+1}) - f(c_i)}{x_{i+1} - c_i}} - \frac{1}{f'(c_i)} \right).
\end{aligned}$$

Expand $f(x_{i+1})$ at c_i as $f(c_i) + f'(c_i)(x_{i+1} - c_i) + f''(\eta)(x_{i+1} - c_i)^2/2$ where η is in the open interval between c_i and x_{i+1} . Then,

$$\begin{aligned}
x_{i+1} - c_{i+1} &= -f^2(c_i) \frac{f''(\lambda)}{2f'(\eta)f'(c_i)} \\
&= -\frac{f'(\tau)^2 f''(\lambda)}{2f'(\eta)f'(c_i)} (c_i - \xi)^2
\end{aligned}$$

where $\tau \in (\min(c_i, \xi), \max(c_i, \xi))$ and $\eta \in (\min(x_{i+1}, c_i), \max(x_{i+1}, c_i))$. Hence, $\{|x_i - c_i|\}_{i=0}^{\infty}$ and $\{|c_i - \xi|\}_{i=0}^{\infty}$ have the same convergence rate around ξ . Now, we study the latter. Again, $f(x_{i+1})$ can be expanded at c_i as $f(c_i) + f'(c_i)(x_{i+1} - c_i) + f''(c_i)(x_{i+1} - c_i)^2/2 + f'''(\kappa)(x_{i+1} - c_i)^3/6$ and $f(\xi) (= 0)$ can be expanded as $f(c_i) + f'(c_i)(\xi - c_i) + f''(\sigma)(\xi - c_i)^2/2$ and $f(c_i) + f'(c_i)(\xi - c_i) + f''(c_i)(\xi - c_i)^2/2 +$

$f'''(\theta)(\xi - c_i)^3/6$. Then, from iteration (4) we have that

$$\begin{aligned}
c_{i+1} - \xi &= \frac{(c_i - \xi)f(x_{i+1}) - (x_{i+1} - \xi)f(c_i)}{f(x_{i+1}) - f(c_i)} \\
&= \frac{x_{i+1} - c_i}{f(x_{i+1}) - f(c_i)}(-f(c_i) + (c_i - \xi) \times \\
&\quad (f'(c_i) + \frac{f''(c_i)}{2}(x_{i+1} - c_i) + \frac{f'''(\kappa)}{6}(x_{i+1} - c_i)^2)) \\
&= \frac{1}{f'(\eta)}(-f(c_i) + (c_i - \xi)f'(c_i) - \\
&\quad \frac{f''(c_i)}{2f'(c_i)}f(c_i)(c_i - \xi) + \frac{f'''(\kappa)f'(\tau)^2}{6f'(c_i)^2}(c_i - \xi)^3) \\
&= \frac{1}{f'(\eta)}(\frac{f''(c_i)}{2f'(c_i)}(c_i - \xi)((c_i - \xi)f'(c_i) - f(c_i)) + \\
&\quad \frac{1}{6}(f'''(\theta) + \frac{f'''(\kappa)f'(\tau)^2}{f'(c_i)^2})(c_i - \xi)^3) \\
&= \frac{1}{f'(\eta)}(\frac{f''(c_i)f''(\sigma)}{4f'(c_i)} + \\
&\quad \frac{1}{6}(f'''(\theta) + \frac{f'''(\kappa)f'(\tau)^2}{f'(c_i)^2}))(c_i - \xi)^3.
\end{aligned}$$

Therefore,

$$\lim_{i \rightarrow \infty} \frac{|c_{i+1} - \xi|}{|c_i - \xi|^3} = \left| \frac{3f''(\xi)^2 + 4f'(\xi)f'''(\xi)}{12f'(\xi)^2} \right|$$

which implies that the sequence $\{c_i - \xi\}_{i=0}^{\infty}$ has at least cubic convergence rate, and so does the interval iteration using (3) and (4). \square

REMARK 5.5. *The efficiency index of algorithms LZ1 and LZ2 are $\sqrt[3]{2}$ and $\sqrt[3]{3}$, respectively. Hence, in the sense of efficiency index LZ2 is also more efficient than LZ1.*

6. SPEED-UP

In this section, we study how to speed up LZ1 and LZ2 by using the floating-point interval method.

As we have seen in Example 5.3, the sizes of the integers representing the intervals increase dramatically. Given $f \in \mathbb{Q}[x]$ and $p/q \in \mathbb{Q}$, then $f(p/q) \in \mathbb{Q}$. In general, the maximal length of the numerator and denominator of $f(p/q)$ approximates to $\deg(f) \max(\text{length}(p), \text{length}(q))$. Hence, if $\deg(f)$ is large, the computation will become quite time and memory consuming.

Numerical computation with floating-point numbers can avoid this difficulty; however, we cannot know exactly whether a numerical result in common sense is reliable or not, i.e., its correct bits is unclear or whether it is zero is unclear.

If floating-point numbers have definite representations, it is possible to estimate the bounds of a numerical result [26, 27, 14, 10]. Hence, for a nonzero real number, a narrow interval with floating-point endpoints can show its correct bits. But zero recognition remains an ill-posed problem.

Note that we have removed all the ill-posed cases in the former sections, i.e., the square-free decomposition to get multiplicities and remove common zeros of f and f' (cf. Section 2), the local monotonic convex decomposition to remove common zeros of f and f'' (cf. Section 4), the restriction $ab > 0$ of input intervals of LZ1 and LZ2 to remove zero roots of $f = 0$ (cf. Section 5). As a result, the floating-point interval method can be applied to evaluate the bounds of

$f(p/q)$ (with Horner scheme) and decide its sign in LZ1 and LZ2.

There exist several packages for the floating-point interval computation, e.g. Rump's `INTLAB/Matlab` package [27, 25], Geulig, Kraemer and Grimmer's `intpack/Maple` package [13] based on the package `intpak/Maple` [12] developed by Corless and Connell, and Revol and Rouillier's MPFI open-source C library [22]. We use the functions in the `intpack/Maple` package, because this package can deal with floating-point numbers with arbitrary lengths and our algorithms need other functions in `Maple`.

To apply the functions in `intpacX`, we should transform LZ1 and LZ2 into their floating-point interval versions and check the computation step by step. Since many similar details should be concerned, it is not suitable to present the pseudo codes here. So we give some principles as follows.

1. Pick the initial length l (decimal digits) of floating-point numbers, e.g. take $l := \max(\min(100, \deg(f) + 5), \text{digits of } a, \text{digits of } b)$.
2. Replace every arithmetic in algorithms LZ1 and LZ2 by corresponding interval arithmetic in `intpacX`.
3. If an interval value of a polynomial at a point contains zero, then increase l (e.g. $l := 2l$ for LZ1) and repeat relative computation until the endpoints of the new interval value share a fixed sign.
4. Rewrite the inequality conditions in the loops and the first lines of the algorithms into interval versions, so that the algorithms can obtain stronger results than in the exact case.

A natural question is whether the super-linear convergence rates can be retained or not when we use the interval method with floating-point numbers instead of exact computation with rational numbers. The answer is "YES". The proof of this claim should deal with many details including why LZ1 and LZ2 can avoid ill-posed cases. We omit most of them and only show the key insight. Suppose that $[u, v]$ is an interval containing ξ and u, v are included in two narrow enough intervals $[u_*, u^*]$ and $[v_*, v^*]$, respectively, where u_*, u^*, v_* and v^* are all floating-point numbers. Then, $\xi \in [u^*, v_*] \subset [u, v]$. To determine whether the two intervals are enough narrow, we should check the signs of the values of the polynomial at the endpoints of $[u_*, u^*]$ and $[v_*, v^*]$. However, $[u_*, v^*]$ is a better choice than $[u^*, v_*]$ in practice, since the former is less possible to obtain a false isolating interval and hence makes the algorithms more efficient than the latter.

EXAMPLE 6.1. *Consider the numerical version of Example 5.3. Take the initial length of floats $l := \max(3+5, \lceil 1.6 \times 8 \rceil) = 12$. Then, the numerical LZ2 yields*

$$\begin{aligned}
[a_0, b_0] &= [4.28515625000, 4.28613281250], \\
[a_0, b_1] &= [4.28515625000, 4.28563130935], \\
[a_1, b_1] &= [4.285631226694662183, 4.28563130935], \\
[a_1, b_2] &= [4.285631226694662183, \\
&\quad 4.28563122670901127793655266277], \text{ and}
\end{aligned}$$

$$(b_2 - a_1)/a_1 = 0.334818704119335811719986541959 \times 10^{-11} < 10^{-8}.$$

To see the convergence rate, we continue to compute

$$[a_2, b_2] = [4.2856312267090112779364772441617276999 \\ 1330501894, 4.28563122670901127793655266277].$$

The correct digits of $[a_1, b_1]$ and $[a_2, b_2]$ are 7 and 22, respectively. This shows that the iteration has cubic convergence rate.

We can find that the expression of b_2 in Example 6.1 is much shorter than that in Example 5.3 and that the swell of coefficients of polynomials has been solved.

7. EXPERIMENTS

To show the effectiveness of the algorithms LZ1 and LZ2, we implemented them in **Maple15** with the open source package **intpakX** [13] and compared our implementations with the **Maple** function **RefineBox** in the package **RegularChains** [5]. All the experiments in this section were done on a computer with Intel(R) Core(TM) i3-2100 CPU @ 3.10GHz.

Chebyshev polynomials of the first kind were used as the tested polynomials and were generated by the **Maple** function **ChebyshevT**. The testing results are listed in Tables 1-4. In each table, L is the number of correct digits of the output (cf. Algorithms 3 and Algorithm 4), “ratio1” and “ratio2” are the rounded time ratios **RefineBox**/LZ1 and **RefineBox**/LZ2, respectively. For each polynomial, we aimed to refining the isolating interval to a precision 10^{-L} . The CPU times in the tables were tested by the **Maple** function **time**.

For a polynomial f with degree n in Table 1, Table 3 and Table 4, we isolated all its real zeros by the function **RealRootIsolate**¹[5] with the option ‘**rerr**’=1/2, picked the $(n/2)$ -th “box”, and refined the isolating interval until its width was no larger than 10^{-5} by **RefineBox**² and viewed the result as the initial isolating interval. For Table 3 and Table 4, this result is [242345/262144, 484695/524288]. Each $(n/2)$ -th “box” happened to contain a zero of the largest irreducible factor g in degree of f and contain no zeros of g' or g'' . We denote the degree of this factor by n^* .

Factorizations for the polynomials in Table 2 were time-consuming. By Algorithm 2, we knew that these polynomials themselves compose their local monotonic convex decompositions. Consequently, they all have monotonic convex isolations according to Definition 4.4. For a polynomial f in Table 2, we used **Isolate** (developed by Fabrice Rouillier in C language) in the **RootFinding** package instead of **RealRootIsolate**, because the former is faster than the latter when n is large and **RefineBox** need not be called for the experiments in this table. The output intervals of **Isolate** with the option **output=interval** were narrow enough that f' and f'' have no zeros and can be used as the input intervals of LZ1 and LZ2. We picked the $(n/2)$ -th element in the output of **Isolate**.

From all of these tables, we can see that our implementations of LZ1 and LZ2 are much faster than the **Maple** function **RefineBox** and in most cases LZ2 was more efficient

¹There are three other methods for isolating real roots in Maple15. They are *realroot*, *RealRootIsolate* with the option *method=Discoverer* [32, 33, 30], and *Isolate* [22, 23, 24] in the *RootFinding* package.

²According to Algorithm 6 in [5], this function performs a generalization of the bisection method; but in this step, it took less than 1 second in all tested cases.

than LZ1. Since the environment variable **Digits** in our implementations of LZ1 and LZ2 did not change continuously, the time costs would have jumps in the tables. Hence, it is not confusing that sometimes LZ1 behaved a little better than LZ2 in our experiments.

Table 1: Timings (s) ($L = 1000$)

n	n^*	RefineBox	LZ1	ratio1	LZ2	ratio2
100	80	89.560	1.965	46	1.794	50
200	160	347.695	4.492	77	3.900	89
300	160	349.317	4.383	80	2.262	154
400	320	1414.819	5.428	261	5.974	237
500	400	2232.982	11.076	202	6.583	309
600	320	1427.814	19.890	72	5.007	285
700	480	3370.198	16.770	201	8.018	420
800	640	5898.132	21.387	276	10.920	540
900	480	3332.259	14.757	226	7.987	417

Table 2: More comparisons ($L = 1000$)

n	1000	1200	1400	1600	1800	2000
LZ1	31.075	27.284	44.928	27.346	59.061	34.398
LZ2	10.888	18.626	15.880	25.958	29.764	33.275

Table 3: Timings (s) ($n = 1000, n^* = 800$)

L	RefineBox	LZ1	ratio1	LZ2	ratio2
100	55.629	5.506	10	3.978	14
200	217.075	9.874	22	5.428	40
300	540.262	11.887	45	5.974	90
400	1067.062	11.934	89	5.787	184
500	1809.892	14.040	129	8.361	216
600	2792.495	13.915	201	12.480	224
700	4103.359	13.884	296	12.558	327

Table 4: More comparisons ($n = 1000, n^* = 800$)

L	800	900	1000	2000	3000
LZ1	14.008	19.578	48.297	48.578	63.679
LZ2	12.448	12.542	12.542	27.705	27.612

8. CONCLUSION

In this paper, we provided a quadratically convergent algorithm LZ1 and a cubically convergent algorithm LZ2 to refine real roots of univariate polynomial equations. Before applying LZ1 or LZ2, the polynomial should be make the square-free decomposition and the local monotonic convex decomposition (LMCD), so that every component polynomial has a monotonic convex isolation (MCI). Moreover, we used the interval method with floating-point numbers to estimate the values of polynomials at rational points to improve the efficiency the algorithms. Experiments on benchmark polynomials showed that if we need high precisions of the real roots, then both of the two algorithms are much faster than the function **RefineBox** in **Maple15**.

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